Generalized Variational Principle for the Scattering Amplitude*

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The Schwinger variational principle in differential form for the S-wave phase shift has been generalized so as to be applicable to the entire scattering amplitude.

VARIATIONAL principles for the calculation of phase shifts in nuclear scattering problems were first introduced by Schwinger[1] and Hulthén[2] and have by now been given numerous other formulations.[3–6] All these depend upon Schrödinger's equation in its differential form. Schwinger[7] has also provided variational principles for both the phase shifts and the scattering amplitude which are based on the integral equation formulation of Schrödinger's equation, but sometimes the use of a varaitional principle involving the differential formulation is more feasible for numerical calculations. The generalization of Hulthén's method for the phase shift to the entire scattering amplitude has been given by Kohn.[8] In the present note it will be shown that a similar generalization exists for the corresponding Schwinger differential formulation.[1] This permits the use of trial functions involving the "inside" wave function[6] representing the difference between the wave function and its asymptotic form.

Let Schrödinger's equation be written as

$$\Delta\psi+k^2\psi-V(r)\psi=0, \tag{1}$$

and let the subscripts 1, 2 denote two particular solutions of Eq. (1) having the asymptotic form

$$\lim_{r\to\infty}\psi_i=e^{i\mathbf{k}_i\cdot\mathbf{r}}+f(\mathbf{k}_i,\mathbf{k})\frac{e^{ikr}}{r},\quad i=1,2. \tag{2}$$

This represents an incident plane wave in the direction $\mathbf{k}_i$ and a scattered wave in the direction $\mathbf{k}$ with amplitude $f(\mathbf{k}_i,\mathbf{k})$. For simplicity, let $\psi_i=e^{i\mathbf{k}_i\cdot\mathbf{r}}+r^{-1}\phi_i$, and form the expression

$$\int d\tau\left(e^{i\mathbf{k}_2\cdot\mathbf{r}}+\frac{1}{r}\phi_2\right)\left(\Delta\frac{\phi_1}{r}+k^2\frac{\phi_1}{r}-V(r)\left[e^{i\mathbf{k}_1\cdot\mathbf{r}}+\frac{\phi_1}{r}\right]\right)=0. \tag{3}$$

By the use of Green's theorem,

$$\int d\tau e^{i\mathbf{k}_2\cdot\mathbf{r}}\left(\Delta\frac{\phi_1}{r}+k^2\frac{\phi_1}{r}\right)=\int dS\left(e^{i\mathbf{k}_2\cdot\mathbf{r}}\frac{\partial}{\partial n}\left(\frac{\phi_1}{r}\right)-\frac{\phi_1}{r}\frac{\partial}{\partial n}e^{i\mathbf{k}_2\cdot\mathbf{r}}\right), \tag{4}$$

where the surface integral extends over an infinitely large sphere. Consequently, the function ϕ_1 may be replaced by its asymptotic form $\chi_1=f(\mathbf{k}_1,\mathbf{k})e^{ikr}$. The resulting expression is readily evaluated[9] and is equal to $-4\pi f(\mathbf{k}_1,-\mathbf{k}_2)$. The terms in Eq. (3) involving ϕ_2 and $\Delta\phi_1$ may be integrated by parts, yielding the symmetric form

$$4\pi f(\mathbf{k}_1,-\mathbf{k}_2)=\int d\tau\frac{1}{r^2}\left\{-\frac{\partial\phi_1}{\partial r}\frac{\partial\phi_2}{\partial r}-\frac{1}{r^2}\frac{\partial\phi_1}{\partial\theta}\frac{\partial\phi_2}{\partial\theta}-\frac{1}{r^2\sin^2\theta}\frac{\partial\phi_1}{\partial\varphi}\frac{\partial\phi_2}{\partial\varphi}+k^2\phi_1\phi_2-V(r)[re^{i\mathbf{k}_1\cdot\mathbf{r}}+\phi_1]\times[re^{i\mathbf{k}_2\cdot\mathbf{r}}+\phi_2]\right\}+\int d\Omega\left[\phi_2\frac{\partial\phi_1}{\partial r}\right]_{r=0}^{r=\infty}. \tag{5}$$

Following Schwinger's analysis, the divergent contribution arising from the evaluation at infinity of the last term above is eliminated by subtracting an exactly similar contribution from the equation for the asymptotic function. Thus, the function χ_1 satisfies the equation

$$\frac{1}{r}\left(\frac{\partial^2}{\partial r^2}\chi_1+k^2\chi_1\right)=0. \tag{6}$$

After multiplying by $r^{-1}\chi_2$ and integrating over all space, one obtains

$$\int d\tau\frac{1}{r^2}\left(-\frac{\partial\chi_1}{\partial r}\frac{\partial\chi_2}{\partial r}+k^2\chi_1\chi_2\right)+\int d\Omega\left[\chi_2\frac{\partial\chi_1}{\partial r}\right]_{r=0}^{r=\infty}=0. \tag{7}$$

Subtracting (7) from (5), one obtains the following

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variational principle for $f(\mathbf{k}_1, -\mathbf{k}_2)$:

$$4\pi f(\mathbf{k}_1, -\mathbf{k}_2)=\int d\tau\frac{1}{r^2}\left\{-\frac{\partial\phi_1}{\partial r}\frac{\partial\phi_2}{\partial r}-\frac{1}{r^2}\frac{\partial\phi_1}{\partial\theta}\frac{\partial\phi_2}{\partial\theta}-\frac{1}{r^2\sin^2\theta}\frac{\partial\phi_1}{\partial\varphi}\frac{\partial\phi_2}{\partial\varphi}+k^2\phi_1\phi_2-V(r)[re^{i\mathbf{k}_1\cdot\mathbf{r}}+\phi_1]\times[re^{i\mathbf{k}_2\cdot\mathbf{r}}+\phi_2]\right\}-\int d\tau\frac{1}{r^2}\left\{-\frac{\partial\chi_1}{\partial r}\frac{\partial\chi_2}{\partial r}+k^2\chi_1\chi_2\right\}+ik\int d\Omega f(\mathbf{k}_1,\mathbf{k})f(\mathbf{k}_2,\mathbf{k}), \quad (8)$$

the last term above being contributed by the last term in Eq. (7). This expression is stationary with respect to arbitrary variations in the functions ϕ_i,χ_i provided that these have the correct radial dependence at infinity, e.g.,

$$\lim_{r\to\infty}\delta\phi_i=\delta\chi_i=\delta f(\mathbf{k}_i,\mathbf{k})e^{ikr}. \quad (9)$$

One can now introduce the "inside" wave function defined by

$$Y_i=\chi_i-\phi_i, \quad (10)$$

which satisfies the boundary conditions

$$Y_i(0)=f(\mathbf{k}_i,\mathbf{k}),\quad Y_i(\infty)=0. \quad (11)$$

Equation (8) may now be written as

$$4\pi f(\mathbf{k}_1, -\mathbf{k}_2)=4\pi f_B(\mathbf{k}_1, -\mathbf{k}_2)+\int d\tau\frac{1}{r^2}\left\{-\frac{\partial Y_1}{\partial r}\frac{\partial Y_2}{\partial r}+k^2Y_1Y_2-\frac{1}{r^2}\frac{\partial}{\partial\theta}(\chi_1-Y_1)\frac{\partial}{\partial\theta}(\chi_2-Y_2)-\frac{1}{r^2\sin^2\theta}\frac{\partial}{\partial\varphi}(\chi_1-Y_1)\frac{\partial}{\partial\varphi}(\chi_2-Y_2)-V(r)[re^{i\mathbf{k}_1\cdot\mathbf{r}}(\chi_2-Y_2)+re^{i\mathbf{k}_2\cdot\mathbf{r}}(\chi_1-Y_1)]\right\}-ik\int d\Omega f(\mathbf{k}_1,\mathbf{k})f(\mathbf{k}_2,\mathbf{k}), \quad (12)$$

where $f_B(\mathbf{k}_1, -\mathbf{k}_2)$ is just the Born approximation

$$4\pi f_B(\mathbf{k}_1, -\mathbf{k}_2)=-\int d\tau e^{i\mathbf{k}_1\cdot\mathbf{r}}V(r)e^{i\mathbf{k}_2\cdot\mathbf{r}}. \quad (13)$$

Equation (12) is stationary with respect to variations in Y_i.

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